Entanglement and Quantum Phase Transitions via Adiabatic Quantum Computation

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For a finite XY chain and a finite two-dimensional Ising lattice, it is shown that the paramagnetic ground state is adiabatically transformed to the GHZ state in the ferromagnetic phase by slowly turning on the magnetic field. The fidelity between the GHZ state and an adiabatically evolved state shows a feature of the quantum phase transition.

I. INTRODUCTION

A quantum computer is a quantum system, so it could simulate quantum dynamics directly and efficiently [1]. When a quantum system undergoes a quantum phase transition (QPT) [2], induced by the variation of external parameters or coupling strength, its ground state changes dramatically and maybe, too, its entanglement. Entangled states, showing quantum correlations between subsystems, are not only valuable resources in quantum information processing but also important for understanding quantum many-body systems. So much attention has been paid to a study of entanglement of quantum many-body systems in ground states or at thermal equilibrium in connection with QPTs [3, 4, 5]. However, the simulation of QPTs and the generation of entangled states with quantum computers are less explored.

In this paper, we address whether QPTs can be simulated with adiabatic quantum computation (AQC) and how the entanglement changes when the QPT takes place. We present a way to generate an entangled state of a quantum system which undergoes a QPT during the quantum adiabatic evolution. As prototypes of QPTs, we consider a spin 1/2 XY chain and a two-dimensional spin 1/2 Ising lattice. It is shown that a product state in the paramagnetic phase is adiabatically transformed to a Greenberg-Horne-Zeilinger (GHZ) entangled state, in the ferromagnetic phase, and *vice versa*. We shows the fidelity between the GHZ state and an adiabatically evolved state could be a good indicator to QPTs. For a two-dimensional Ising model, *a two-dimensional* GHZ state is generated via AQC.

II. ADIABATIC QUANTUM COMPUTATION

Let us start with a brief introduction to AQC [6]. Quantum computation can be implemented by the controlled dynamics of quantum states governed by the Schrödinger equation with a time-dependent Hamiltonian

$$i\hbar \frac{d}{dt}|\Psi(t)\rangle = H(t)|\Psi(t)\rangle \,, \qquad (1)$$

and quantum measurements. In a quantum circuit model, the evolution of a quantum state is decomposed into a series of single-qubit and two-qubit gates, which can be implemented by applying external pulses and by controlling the interaction between two qubits. On the other hand, AQC relies on the adiabatic theorem, which states that an evolved quantum system will stay at its instantaneous eigenstate if the time-dependent Hamiltonian changes very slowly. If the Hamiltonian $H(t)$ in Eq. (1) changes slowly, then the initial state $|\Psi(0)\rangle$, taken as an eigenstate state $|\varphi_n(0)\rangle$ of an initial Hamiltonian $H(0) \equiv H_0$ at $t = 0$, evolves to $|\Psi(T)\rangle = |\varphi_n(T)\rangle$, an eigenstate of a problem Hamiltonian $H(T) \equiv H_P$ at $t = T$. The run time T is inversely proportional to the square of the minimum energy gap during the evolution. It is convenient to introduce the dimensionless time $s \equiv t/T$ with $0 \leq s \leq 1$. There are many ways to connect H_0 and H_P smoothly as a function of s, for example, simple linear or nonlinear interpolations [7]. A general interpolation is given by $H(s) = f(s)H_0 + g(s)H_P$ where two functions $f(s)$ and $g(s)$ satisfy the boundary conditions, $f(0) = g(1) = 1$ and $f(1) = g(0) = 0$. It is known that a proper interpolation could reduce the run time of AQC.

III. ENTANGLEMENT AND QPTS OF THE XY CHAIN VIA AQC

The Hamiltonian of a spin 1/2 XY chain in a transverse magnetic field is written as

$$H_{XY} = - \sum_{i=1}^{N} \left[\left(\frac{1+\gamma}{2} \right) \sigma_i^z \sigma_{i+1}^z + \left(\frac{1-\gamma}{2} \right) \sigma_i^y \sigma_{i+1}^y \right]$$
$$- \lambda \sum_{i=1}^{N} \sigma_i^x \,, \qquad (2)$$

where N is the total number of spins, λ the transverse magnetic field, and γ the parameter for the degree of anisotropy of spin-spin interaction. Here, the coordinates x and z are exchanged for convenience as in

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Ref. [2]. The periodic boundary condition, $\sigma_{N+1} = \sigma_1$, is assumed. For $\gamma = 1$, it becomes the Ising model $H_I = -\sum_{i=1}^{N} \sigma_i^z \sigma_{i+1}^z - \lambda \sum_i \sigma_i^x$. For $\gamma = 0$, it is called the XX model.

Let us recall the ground state of the Ising model which undergoes the QPT at $\lambda_c = 1$ [2]. If $\lambda \gg 1$, the Zeeman term in Eq. (2) is dominant and the ground state is given by the product of eigenstates of σ_i^x, called the paramagnetic state

$$|P\rangle \equiv \prod_{i=1}^{N} |+\rangle_i\,, \qquad (3)$$

where $|+\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$. In the other limit of $\lambda \ll 1$, the spin-spin interaction in Eq. (2) is important and the ground state has two-fold degeneracy. A possible ground state can be any superposition of all spin up state $|F_\uparrow\rangle$ and all spin down state $|F_\downarrow\rangle$ where

$$|F_\uparrow\rangle \equiv \prod_{i=1}^{N} |\uparrow\rangle_i\,, \quad |F_\downarrow\rangle \equiv \prod_{i=1}^{N} |\downarrow\rangle_i\,. \qquad (4)$$

One possible ground state is the GHZ state of N spins

$$|\mathrm{GHZ}\rangle_N = \frac{1}{\sqrt{2}}(|F_\uparrow\rangle + |F_\downarrow\rangle)\,. \qquad (5)$$

In the thermodynamic limit, $N \to \infty$, the ground could be either $|F_\downarrow\rangle$ or $|F_\uparrow\rangle$ due to the spontaneous symmetry breaking. However, a computer resource is *finite* no matter whether it is classical or quantum. So we focus on the adiabatic quantum simulation of QPTs and the generation of entangled states with a finite system.

The spin 1/2 XY chain is exactly solvable in the sense that its energy spectrum, ground state, and phase diagram can obtained via the mapping of spin operators to fermion operators via the Jordan-Wigner transformation [8, 9]. Recently, this system has attracted much attention in the study of the relation between entanglement and QPTs. Osborne and Nielsen [4] studied the entropy of a single spin and the two-spin entanglement, where $|F_\uparrow\rangle$ was taken as a ground state in the ferromagnetic phase. Osterloh *et al.* [3] investigated the two spin entanglement of the spin 1/2 XY chain and showed that the concurrence as a two-spin entanglement measure exhibits the characteristic features of QPTs. Note that both $|F_\uparrow\rangle$ and $|\mathrm{GHZ}\rangle_N$ have the same value of the two-spin entanglement, i.e., zero concurrence, although $|P\rangle$, $|F_\uparrow\rangle$, and $|F_\downarrow\rangle$ are separable states but $|\mathrm{GHZ}\rangle_N$ is entangled. The behavior of multi-particle entanglement at QPTs is an open problem because a good entanglement measure for more than two spins is still under development [10, 11, 12, 13]. The direct simulation of QPTs via AQC might give a clue to this problem.

For the simulation of QPTs of the XY model via AQC, let us decompose the Hamiltonian H_{XY} into two parts: the initial Hamiltonian H_0 and the problem Hamiltonian
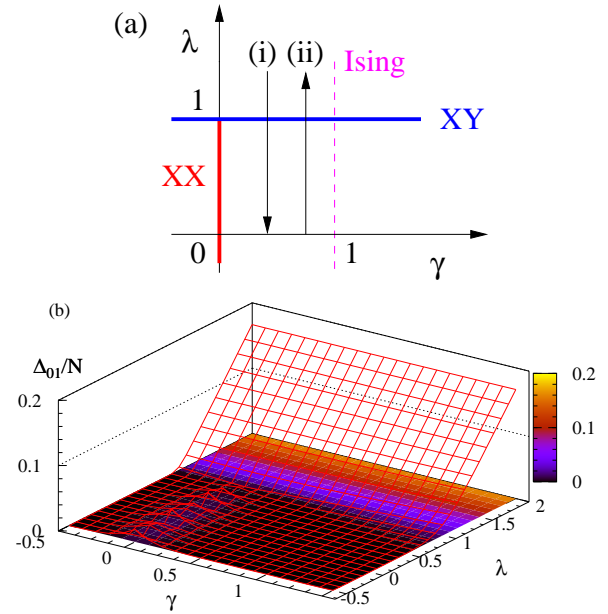

FIG. 1: (a) Phase diagram of the XY chain with the XY critical line at $\lambda = 1$ and the XX critical line at $\gamma = 0$ [9]. It is symmetric about γ and λ axes. Path (i) starts from the paramagnetic phase and end at the ferromagnetic phase. The return path is denoted by (ii). (b) Energy gap Δ_{01}/N between the two lowest eigenvalues as a function of γ and λ.

H_P

$$H_0 = -\sum_{i=1}^{N} \sigma_i^x\,, \quad H_P(\gamma) = H_{XY} - \lambda H_0\,. \qquad (6)$$

Among various ways of connecting H_0 and H_P, two interpolation schemes, linear and square ones, are considered to see whether a proper interpolation could reduce the run time of AQC. The linear interpolation is given by

$$H_{XY}(s, \gamma) = (1-s)H_0 + sH_P(\gamma)\,, \qquad (7)$$

and the square interpolation reads

$$H_{XY}(s, \gamma) = (1-s^2)H_0 + s(2-s)H_P(\gamma)\,, \qquad (8)$$

By comparing of Eqs. (2), (7), and (8), one obtains the time-dependence of the magnetic field $\lambda(s) = (1-s)/s$ for the linear interpolation, and $\lambda(s) = (1-s^2)/(2s-s^2)$ for the square interpolation. The path of adiabatic evolution from the paramagnetic phase to the ferromagnetic phase is depicted in Fig. 1 (a). At time $s = 0$ corresponding to the limit $\lambda \to \infty$, the initial state is given by the paramagnetic state, Eq. (3). At $s = 1/2$, i.e., $\lambda = 1$, the system arrives at the XY critical line. The adiabatic evolution ends at $s = 1$, that is, $\lambda = 0$. We examine which of two states, Eqs. (4) and (5) is the true final state by calculating the fidelity between the GHZ state and an evolved state as function of s and γ. Note that

Wei *et al.* [14] used the maximum fidelity between a state and an untangled state as a global entanglement measure in the study of the multi-particle entanglement of a XY chain. To check the reversibility of AQC, we investigate the reverse path from the ferromagnetic phase, starting with (4) or (5), to the paramagnetic phase by exchanging H_0 and H_P.

For the numerical simulation of the AQC, we develop the program which solves the Schrödinger equation and diagonalizes the Hamiltonian directly without the Jordan-Wigner transformation. We simulate the spin $1/2$ XY chain with $N = 12$, and a two-dimensional Ising model of size 3×3 on a personal computer.

For the one-dimensional XY model, the energy spectrum is obtained as function of λ and the anisotropy parameter γ as shown in Fig. 1 (b). As the free energy determines classical phase transitions, the energy gap between the ground state and the first exited state plays a key role in QPTs. As depicted in Fig. 1 (b), the gap Δ_{01} between the two lowest eigenvalues of the XY Hamiltonian clearly vanishes at the critical line, i.e., at $\lambda = 1$. On this line the two lowest eigenvalues merge together and the ground state becomes degenerate, even though the system size is finite.
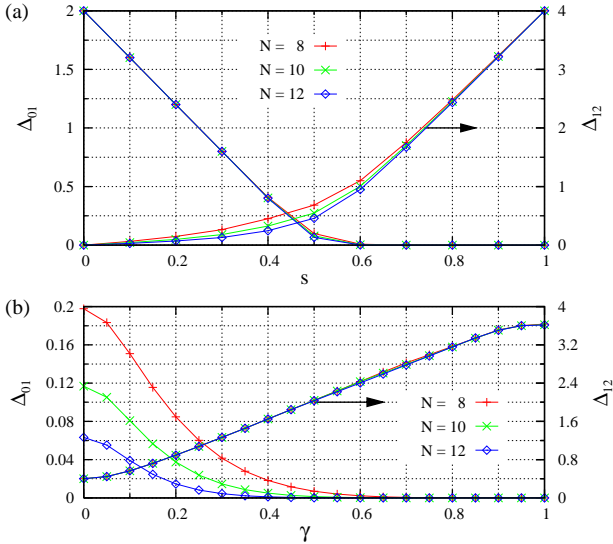

FIG. 2: (a) Δ_{01} and Δ_{12} as a function of s at $\gamma = 1$ for $N = 8, 10, 12$. (b) Δ_{01} and Δ_{12} as a function of γ at $\lambda = 0.1$ for $N = 8, 10, 12$. The linear interpolation is used.

Fig. 2 (a) plots Δ_{01} and Δ_{12}, the gap between the second and third lowest eigenvalues, as a function of s at $\gamma = 1$ for $N = 8, 10, 12$. Δ_{01} is nearly independent of N. However, Δ_{12} is more dependent on N near the critical points $s_c = 1/2$, i.e., $\lambda_c = 1$. The energy gap Δ of the spin $1/2$ XY chain with infinite size is known to be $\Delta \sim |\lambda - \lambda_c|$ [2]. Δ_{01} and Δ_{12} can be regarded as the energy gaps between the ground state and the first excited state in the paramagnetic phase and in the ferromagnetic phase, respectively. That is $\Delta(\lambda) = \Delta_{01}(\lambda)$ for $\lambda > 1$ and

$\Delta(\lambda) = \Delta_{12}(\lambda)$ for $\lambda < 1$. So the critical slowing down at the critical point [16] is due to Δ_{12} not due to Δ_{01} as $N \to \infty$. Let us examine the universality of Δ_{01}, that is, independent of γ. Due to the finite size effect, the region of the universality defined by $\Delta_{01} = 0$ does not extend to the XX line, i.e., $0 < \gamma \leq 1$ for the infinite lattices. The region satisfying the universality grows with N as shown in Fig. 2 (b).
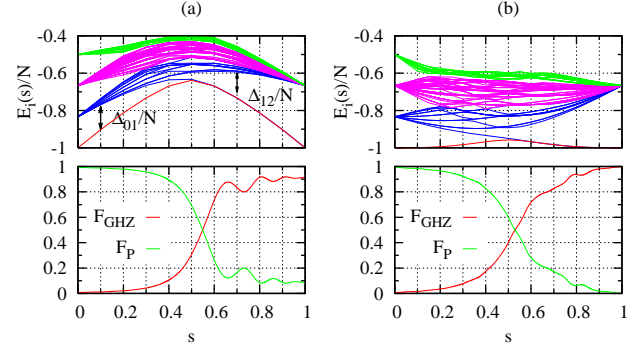

FIG. 3: Energy levels per spin and the fidelity as a functions of s for the XY model with $N = 12$ and $\gamma = 0.75$ (a) for the linear interpolation, and (b) for the square interpolation. The run time $T = 20$ is taken. The energy spectrum ranges from -1 to 1 and is symmetric about x axis.

Fig. 3 shows the difference between the linear interpolation and the square interpolation. The linear interpolation needs more run time T, than the square one. The main reason is that the gap Δ_{12} for the square interpolation is larger at the critical region than that for the linear one, so the probability for the transition to the excited states is reduced. We find that the square interpolation could reduce the run time T of AQC in the case of the XY chain.
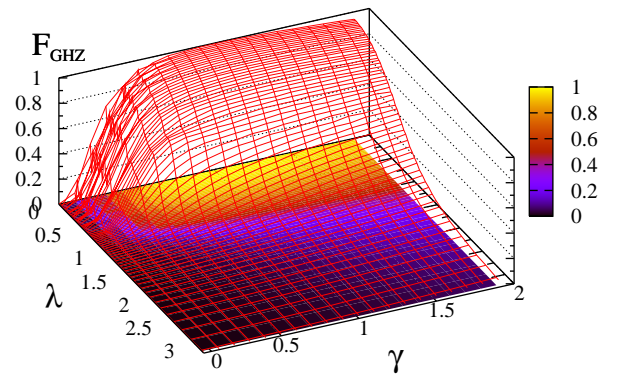

FIG. 4: Fidelity F_{GHZ} between the GHZ state and the evolved state as a function of $\lambda(s)$ and γ. $N = 10$, $T = 20$, and the square interpolation are used.

Fig. 4 shows the fidelity between an evolved state and the GHZ state, $F_{\text{GHZ}}(s) = |\langle \Psi(s) | \text{GHZ} \rangle|^2$, as a function

of s and γ. The paramagnetic state $|P\rangle$ in Eq. (3) at $s = 0$ ($\lambda \gg 1$) adiabatically evolves to the GHZ state $|\text{GHZ}\rangle_N$ in Eq. (5) at $s = 1$ ($\lambda = 0$). Especially, at $\gamma = 1$, this result is consistent with Dorner et al.'s one [15]. They showed that for the Ising chain the paramagnetic state is transformed to the GHZ state by slowly decreasing the magnetic field λ. Although due to the finite size effect, the fidelity decreases near the XX critical line, it is almost independent of of γ. This is one of the characteristic features of QPTs, called the universality. As mentioned before, the region of the universality is dependent on the number of spins N.

Let us discuss the reversibility of the QPT. The paramagnetic state is adiabatically transformed to the GHZ state in the ferromagnetic phase by decreasing λ. Does the GHZ state evolve adiabatically to the paramagnetic state (3) even though there is the energy level splitting at the XY critical line? By exchanging H_0 and H_P, the reverse evolution, the return path (ii) in Fig. 1 (a), can be implemented. To examine the reversibility of AQC, let us consider $H_{XY}(s, \gamma) = f(s)H_0 + g(s)H_P(\gamma)$ where $f(s) = 4(s - 1/2)^2$ and $g(s) = -4s(s - 1)$. At $s = (2 - \sqrt{2})/4$, the paramagnetic to ferromagnetic transition happens. The ferromagnetic to paramagnetic transition takes place at $s = (2 + \sqrt{2})/4$. We find that in spite of the energy level merging and splitting during the journey, the paramagnetic state is adiabatically transformed to the GHZ state and vice versa as shown in Fig. 5 (b).
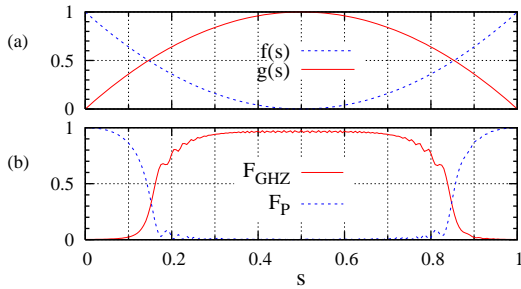

FIG. 5: (a) Two functions $f(s)$ and $g(s)$ as a function s for the round trip. (c) F_{GHZ} and F_P as a function of s with $\gamma = 0.8$, $N = 10$, $T = 200$.

Let us discuss the effect of finite system size on the AQC simulation of QPTs and the generation of entangled states. Although the system considered here is finite, it could show important features of QPTs. First, QPTs are characterized by the energy level crossing or avoided crossing [2]. Fig. 1 (b) shows energy level crossings at $\lambda = 1$. Second, a XY spin chain exhibits the universality, which state that the physics is independent of γ for $0 < \gamma \leq 1$. The energy gap in Figs. 1 (b) and the fidelity in Fig. 4 are independent of γ, although the universality is not perfect due to the finite size effects. Third, Fig. 4 shows the abrupt change in the ground state at QPT. One unsolved issue is that the entanglement of the ground state in the ferromagnetic phase. If either $|F_\uparrow\rangle$ or

$|F_\downarrow\rangle$ is the ground state in the ferromagnetic phase, there is no entanglement. On the other hand, the ground state $|\text{GHZ}\rangle_N$ is a multi-particle entangled state. In this case, the single-site entropy varies from 0 at the paramagnetic phase to 1 in the ferromagnetic phase. This is in contrast with the result of [4]. A related question is whether the entanglement of the ground state in ferromagnetic or paramagnetic phase is constant or dependent on λ. In other words, does entanglement change abruptly only at the critical point?

IV. ENTANGLEMENT OF TWO-DIMENSIONAL ISING MODEL

Let us turn to the two-dimensional Ising model to produce the two-dimensional GHZ state

$$|\text{GHZ}\rangle_{2D} = \frac{1}{\sqrt{2}} \left(\prod_{i,j=1}^{N} |\uparrow\rangle_{ij} + \prod_{i,j=1}^{N} |\uparrow\rangle_{ij} \right), \qquad (9)$$

where $|\uparrow\rangle_{ij}$ is the spin-up state at the lattice site i and j. As illustrated in Fig. 6 (a), the 3×3 two-dimensional lattice is considered. The open boundary condition is assumed. The two-dimensional Ising model can be mapped to the one-dimensional Ising model with long-range interactions as depicted in Fig. 6 (a). Fig. 6 (b) and (c) show several lowest energy levels, and the fidelity between an evolved state and the two-dimensional GHZ state defined by Eq. (9) as a function of s. Like one-dimensional spin 1/2 XY model, the two dimensional GHZ state can be generated via AQC.
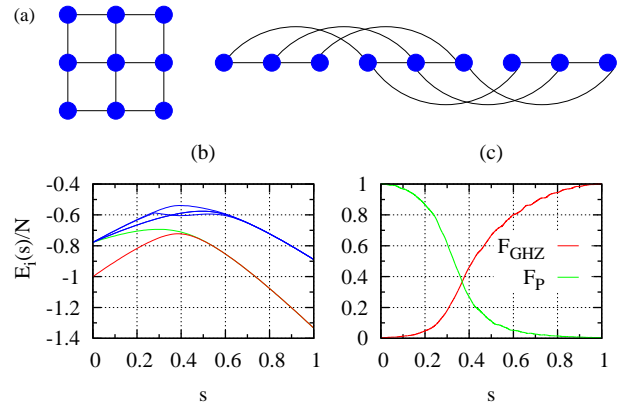

FIG. 6: Two dimensional square lattice of size 3×3 and its mapping to the one-dimensional lattice with long-range interaction. (b) Energy levels as a function of s with the linear interpolation. (c) Fidelity between the evolved state and the two-dimensional GHZ state as a function of s.

V. SUMMARY

We have considered the one-dimensional XY model and the two-dimensional Ising model and simulated the

QPTs and the generation of an entangled state via AQC. Although the system size is finite, our results show the characteristic features of QPTs. It has been demonstrated that the paramagnetic state evolves adiabatically to the GHZ state in the ferromagnetic phase and vice versa. The generation of entangled states via AQC is simple in the sense that only the external magnetic field is turned off or on slowly. It doesn't require the control of the exact qubit-qubit coupling, i.e., CNOT gate. We have shown that a square interpolation scheme is better in reducing the run time than linear one.

One open issue in AQC is that the minimum energy gap, which determine the run time T, should be known before running. Also the run time should be smaller than the decoherence time but at the same time large enough to avoid the unwanted transition. We are studying the effect of decoherence on AQC by solving the Lindblad master equation [17] and the generation of W-type entangled states or cluster states [18] via AQC. Also, it is interesting to study how to simulate a quantum system in the thermodynamic limit with finite quantum computational resources.

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